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Coupling atomistic and continuum modelling of magnetism

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Abstract

In this article, a new energy-based atomistic-continuum partitioned-domain multiscale method for magnetisation dynamics is proposed. The main feature of the method is the minimised mismatch between the local continuum description and the non-local atomistic description (in which non-nearest neighbour interatomic interactions are present). The error at the atomistic-continuum interface is minimised by constructing an intermediate region consisting of *transition atoms*, which interact differently with the neighbouring atomistic and continuum regions. When the mesh of the continuum region is refined to the atomistic scale at the atomistic-continuum interface and an energy-conserving time-stepping scheme is used for the entire computational domain, the method conserves the total energy of the system. The second feature of the method is the introduction of a *damping band* at the atomistic-continuum interface, which absorbs high-frequency waves that are otherwise reflected from the interface and thereby contribute to the error inside the atomistic region. Several examples of domain wall motion and spin wave propagation in one- and two-dimensional structures are used to illustrate the applicability of the method and to investigate its limitations.

Keywords: magnetisation dynamics, multiscale modelling,

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